Observation of the Nuclear Magnetic Octupole Moment of ^{87}Rb from Spectroscopic Measurements of Hyperfine Intervals

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The magnetic octupole moment of ^{87}Rb is determined from hyperfine intervals in the $5p\ ^2P_{3/2}$ state measured by Ye et al. [Opt. Lett. **21**, 1280 (1996)]. Hyperfine constants $A = 84.7189(22)$ MHz, $B = 12.4942(43)$ MHz, and $C = -0.12(09)$ kHz are obtained from the published measurements. The existence of a significant value for C indicates the presence of a nuclear magnetic octupole moment Ω. Combining the hyperfine constants with atomic structure calculations, we obtain $\Omega = -0.58(39)$ bμ_N. Second-order corrections arising from interaction with the nearby $5p\ ^2P_{1/2}$ state are found to be insignificant.

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I. INTRODUCTION

We report values of the nuclear magnetic octupole moment of ^{87}Rb determined from measured hyperfine intervals. During an earlier investigation of the hyperfine structure of atomic ^{133}Cs [1], we discovered existing measurements of the hyperfine structure of the $5p\ ^2P_{3/2}$ state of ^{87}Rb ($I = 3/2$, $F = 0, 1, 2, 3$) by Ye et al. [2] with a frequency resolution of several kHz. The measured hyperfine intervals $\Delta W_F = W_F - W_{F-1}$ are shown in Fig. 1. These intervals were decomposed in terms of nuclear magnetic dipole and electric quadrupole coupling coefficients (A and B) in Ref. [2] and the resulting values for A and B are given in the first row of Table I. However, for an atomic state with angular momentum $J \geq 3/2$, there also exists a coupling between the nuclear magnetic octupole moment and the electronic state, provided $I \geq 3/2$. Precision measurements of the three hyperfine intervals in ^{87}Rb are sufficient to determine three hyperfine constants A, B and C, representing the interaction of the nuclear magnetic dipole moment μ_I, electric quadrupole moment Q, and magnetic octupole moment Ω, respectively, with the atomic electrons. We combine the coefficient C, determined herein, with atomic structure calculations for neutral ^{87}Rb to determine the nuclear octupole moment. The purpose of the present paper is to determine the previously unknown nuclear magnetic octupole moment of ^{87}Rb, not to discuss the experimental work by Ye et al..

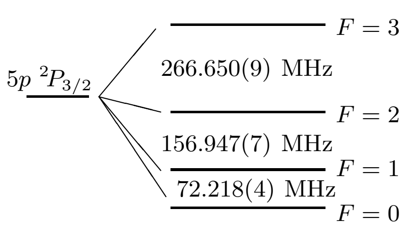

FIG. 1: Hyperfine structure of the $5p\ ^2P_{3/2}$ state in ^{87}Rb from Ye et al. [2].

The (unperturbed) hyperfine structure intervals of an atom having a single electron outside closed shells and $I = J = 3/2$ is given in terms of the hyperfine constants A, B and C by [3]

$$\Delta W_3 = 3A + B + 8C \tag{1}$$
$$\Delta W_2 = 2A - B - 28C \tag{2}$$
$$\Delta W_1 = A - B + 56C. \tag{3}$$

Inverting these equations leads to the values of A, B and C given in the second row of Table I.

II. SEMI-EMPIRICAL ANALYSIS

With the aid of approximations developed by Casimir [4], semi-empirical estimates for the hyperfine coupling constants can be expressed in terms of the nuclear moments μ_I, Q, and Ω of ^{87}Rb. To evaluate the hyperfine constants empirically, we start from the nonrelativistic expressions for A, B and C [3, Chap. VIII], which can be written

$$A(5p_{3/2}) = \mu_I(\mu_N)\,\frac{16}{45}\left\langle\frac{1}{r^3}\right\rangle_{5p} F \times 95.4107\ \text{MHz} \tag{4}$$

$$B(5p_{3/2}) = Q(b)\,\frac{2}{5}\left\langle\frac{1}{r^3}\right\rangle_{5p} R \times 234.965\ \text{MHz} \tag{5}$$

$$C(5p_{3/2}) = \Omega(\mu_N b)\,\frac{2}{35}\left[\frac{R^2_{5p}(r)}{r^4}\right]_0 T \times 3.40718\ \text{Hz}. \tag{6}$$

The atomic matrix elements in Eqs. (4,5) are expressed in atomic units. In Eq.(6), $R_{5p}(r)$ is the radial wave

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TABLE I: Hyperfine coupling constants A, B and C from measured hyperfine intervals of ^{87}Rb $5p\ ^2P_{3/2}$. First row: results obtained by Ye et al. [2], second row: present analysis, third row: semi-empirical estimates, fourth row: MBPT results. In the semi-empirical and MBPT calculations, we use $\mu_I = 2.7516\mu_N$ from Raghavan [6] and $Q = 133.5(5)$ mb from Pyykkö [7]. Ω is expressed in μ_Nb.

	A (MHz)	B (MHz)	C (kHz)
Ref. [2]	84.7185(20)	12.4965(37)	
Present Work	84.7189(22)	12.4942(43)	-0.12(09)
Semi-empirical	91.4	12.5	0.293 Ω
MBPT	83.0	12.6	0.206 Ω

function of the $5p$ state and, again, atomic quantities are expressed in atomic units. The factors F, R, T in the above equations account for relativistic effects. With aid of the Casimir approximations, we write

$$\left\langle \frac{1}{r^3} \right\rangle_{np} \approx \frac{Z_i^2 Z}{3(n^*)^3}\left(1-\frac{d\sigma}{dn}\right) = 0.95983\, a_0^{-3} \tag{7}$$

$$\left[\frac{R_{np}^2(r)}{r^4}\right]_0 \approx \frac{4Z_i^2 Z^3}{9(n^*)^3}\left(1-\frac{d\sigma}{dn}\right) = 1393.68\, a_0^{-5}. \tag{8}$$

In the above expressions, $Z = 37-4 = 33$ is the effective nuclear charge [3, p. 166], $Z_i = 1$ is the ionic charge, n^* is the effective quantum number of the $5p_{3/2}$ state, and σ is the quantum defect. From Van Wijngaarden [5], we find $n^* = 2.293$ and $d\sigma/dn = -0.052$, for the $5p_{3/2}$ state of Rb. Using the values $\mu_I = 2.7516\mu_N$ [6] and $Q = 0.1335\ b$ [7] for ^{87}Rb, we obtain

$$A(5p_{3/2}) \approx 89.6\, F \text{ MHz} \tag{9}$$

$$B(5p_{3/2}) \approx 12.0\, R \text{ MHz} \tag{10}$$

$$C(5p_{3/2}) \approx 0.271\, T\ \Omega \text{ kHz}. \tag{11}$$

We estimate the relativistic correction factors F, R, T by comparing relativistic and nonrelativistic Hartree-Fock (HF) calculations of A, B and C. In this way, we obtain $F = 1.02$, $R = 1.04$, and $T = 1.08$. The semi-empirical values listed in Table I include these relativistic corrections. As seen from the table, the semi-empirical value for A differs from experiment by 8%, while the value of B differs by less than 0.1%.

III. RELATIVISTIC MANY-BODY ANALYSIS

In Ref. [8], a relativistic many-body method, referred to as the SD approximation, in which single and double excitations of Dirac-Hartree-Fock wave functions are iterated to all orders in perturbation theory, was used to predict magnetic-dipole hyperfine constants for low-lying states of alkali-metal atoms to within a few percent. The SD value for the magnetic-dipole hyperfine constant of the $5p_{3/2}$ state of ^{85}Rb from [8] is $A = 24.5$ MHz. This value is scaled by the ratio

$$\frac{g_I[^{87}\text{Rb}]}{g_I[^{85}\text{Rb}]} = \frac{2.7516/(3/2)}{1.3534/(5/2)} = 3.3885$$

giving $A = 83.0$ MHz for the $5p_{3/2}$ state of ^{87}Rb shown in the fourth row of Table I. The all-order method described in [8] was used here to obtain $B/Q = 94.16$ MHz and $C/\Omega = 0.206$ kHz, leading to the values of B and C listed in the fourth row of Table I. The theoretical uncertainty in these values is estimated to be 2%.

Experimental values of the nuclear moments are listed in the first row of Table II. By comparing the all-order SD values of A/μ_I and B/Q with the experimental values of A, B and C shown in the second-row of Table I, we obtain the MBPT values of nuclear moments μ_I, Q given in the second row of Table II. The values of μ_I and Q determined in this way agree to within 2% with precise measurements. Comparing the theoretical value of C/Ω with the experimental value of C given in the second row of Table I leads to the principal prediction of the present paper: Ω = -0.58(39) μ_Nb.

IV. ESTIMATING NUCLEAR MOMENTS

It is of interest to compare values of nuclear moments inferred from atomic structure calculations with values obtained directly from nuclear shell-model calculations. In the extreme shell model [9], properties of ^{87}Rb can be described assuming a single valence nucleon moving around an inert core. According to Schwartz [10], the shell-model predictions for the nuclear moments μ_I, Q and Ω are:

$$\mu_I = \mu_N I \times \left\{ \begin{array}{ll} g_L + (g_S - g_L)/(2I), & I = L + 1/2 \\ g_L - (g_S - g_l L)/(2I+1), & I = L - 1/2 \end{array} \right. \tag{12}$$

$$Q = -\frac{2I-1}{2I+2} g_L \langle r^2 \rangle \tag{13}$$

$$\Omega = \frac{2}{3}\mu_N \frac{(2I-1)}{(2I+4)}\langle r^2 \rangle \times \left\{ \begin{array}{ll} (I+2)[(I-3/2)g_L + g_S], & I = L + 1/2 \\ (I-1)[(I+5/2)g_L - g_S], & I = L - 1/2 \end{array} \right. . \tag{14}$$

For ^{87}Rb, the unpaired $p_{3/2}$ proton has total angular momentum $I = 3/2$, orbital angular momentum $L = 1$, and spin angular momentum $S = 1/2$. The proton spin gyromagnetic ratio is $g_S = 5.585694701(56)$ [11] and the orbital gyromagnetic ratio is $g_L = 1$. Using the value of the mean-squared nuclear radius $\langle r^2 \rangle = 0.180$ b from [12], we obtain the values of the three nuclear moments given in the third row of Table II. Comparing the shell-model value of Q with the experimental value shown in

TABLE II: Nuclear moments of ^{87}Rb. First row: mean experimental values, second row: values calculated using MBPT matrix elements and the hyperfine constants given in Table I, third row: values calculated in the extreme nuclear shell model Eqs.(12-14).

	μ_I (μ_N)	Q (mb)	Ω (μ_Nb)
Expt.	2.751639(2)	133.5(5)	-
MBPT	2.70	135	-0.58(39)
Shell-model	3.79	-72	0.30

Table II, it is clear that nuclear many-body effects modify both sign and magnitude of the shell-model prediction. Therefore, the difference in sign and magnitude between the value of Ω predicted here and given in the second row of Table II and the shell-model value shown in the third row is not particularly surprising!

V. SECOND-ORDER CORRECTIONS

Second-order hyperfine corrections will modify Eqs. (1-3) and possibly influence the value of C extracted from these equations. In this section, we investigate the influence of second-order corrections and show that they have a negligible effect on the $5p_{3/2}$ hyperfine constants in ^{87}Rb. The second-order correction to the energy of a state $|0\rangle$ can be written

$$W^{(2)} = \sum_n \frac{\langle 0|H_{\rm hf}|n\rangle\langle n|H_{\rm hf}|0\rangle}{E_0 - E_n}, \tag{15}$$

where $H_{\rm hf}$ is the hyperfine interaction Hamiltonian. For the case of interest here, $|0\rangle$ is a particular hyperfine substate of the $5p_{3/2}$ state and the sum over states $|n\rangle$ is restricted to substates of the nearby $5p_{1/2}$ state. Only the two substates $F = 1$ and $F = 2$ of the $5p_{3/2}$ states are modified by interaction with the $5p_{1/2}$ state. Following the discussion in [13], we find

$$W_F^{(2)} = \begin{cases} \frac{1}{36}\eta - \frac{\sqrt{5}}{60}\zeta & \text{for } F{=}1 \\ \frac{1}{20}\eta + \frac{\sqrt{5}}{100}\zeta & \text{for } F{=}2, \end{cases} \tag{16}$$

where

$$\eta = \mu_I^2\, \frac{20}{3}\, \frac{\langle 5p_{3/2}\|T_1\|5p_{1/2}\rangle^2}{\Delta E} \tag{17}$$

$$\zeta = \mu_I Q\, \frac{20\sqrt{3}}{3}\, \frac{\langle 5p_{3/2}\|T_1\|5p_{1/2}\rangle\langle 5p_{3/2}\|T_2\|5p_{1/2}\rangle}{\Delta E}. \tag{18}$$

The magnetic dipole operator T_1 and electric quadrupole operator T_2 in the atomic reduced matrix elements in the numerators of Eqs.(17) and (18) are defined in [14, Chap. V], and the energy denominator ΔE in Eqs.(17) and (18) is the $5p_{3/2} - 5p_{1/2}$ fine-structure interval. Relativistic many-body calculations carried out in the SD approximation [8] give

$$\langle 5p_{3/2}\|T_1\|5p_{1/2}\rangle = 22.3 \text{ MHz}/\mu_N$$
$$\langle 5p_{3/2}\|T_2\|5p_{1/2}\rangle = 219.6 \text{ MHz/b}.$$

The $5p$ fine-structure interval in ^{87}Rb is ΔE = 7,123,020.80(5) MHz [15]. Combining these values, we find $\eta = 3.524$ kHz and $\zeta = 2.916$ kHz.

Including second-order corrections, Eqs. (1-3) become

$$\Delta W_3 = 3A + B + 8C - \frac{1}{20}\eta - \frac{\sqrt{5}}{100}\zeta \tag{19}$$

$$\Delta W_2 = 2A - B - 28C + \frac{1}{45}\eta + \frac{2\sqrt{5}}{75}\zeta \tag{20}$$

$$\Delta W_1 = A - B + 56C + \frac{1}{36}\eta - \frac{\sqrt{5}}{60}\zeta. \tag{21}$$

Inverting these equations leads to the following second-order corrections to the previously determined values of A, B and C listed in the second row of Table I:

$$A^{(2)} = \frac{1}{180}\eta - \frac{\sqrt{5}}{750}\zeta = 0.0000109 \text{ MHz} \tag{22}$$

$$B^{(2)} = \frac{1}{30}\eta + \frac{\sqrt{5}}{100}\zeta = 0.000183 \text{ MHz} \tag{23}$$

$$C^{(2)} = \frac{\sqrt{5}}{2000}\zeta = 0.00326 \text{ kHz}. \tag{24}$$

The above equations for the second-order corrections are in precise agreement with results for ^{87}Rb presented by Beloy and Derevianko in Ref. [16]. The second-order corrections leave the experimental values of A and C listed in the second row of Table I unchanged and insignificantly increase the value of B to 12.4944(43) MHz.

VI. CONCLUSIONS

In summary, the precise hyperfine measurements of the $5p_{3/2}$ hyperfine interval in ^{87}Rb by Ye et al. [2] are reanalyzed, allowing for the possibility of a nonvanishing nuclear magnetic octupole moment. Assuming that second-order effects in the hyperfine interaction are negligible, we obtain the values listed in the second row for the hyperfine constants A, B and C. In particular, we find a nonzero value for $C = -0.12(09)$ MHz. Values of A/μ_I, B/Q and C/Ω are evaluated both empirically and using relativistic all-order methods. The empirical calculations in combination with the experimental measurements lead to values of μ_I and Q that agree with other measured values to better than 8%, while the all-order calculations combined with the experimental hyperfine constants lead to values of μ_I and Q that agree with other measurements at the 2% level. With the aid of all-order calculations, we infer the value $\Omega = -0.58(39)$ μ_nb for the nuclear magnetic octupole moment. This value (together with

the measured value of Q) is larger in magnitude and different in sign than the value predicted by the nuclear shell model. We examined the influence of the second-order hyperfine corrections arising from the interaction between the $5p_{3/2}$ state and the neighboring $5p_{1/2}$ state. These corrections are found to make insignificant changes in the values of A, B and C extracted from the measurements. Inasmuch as the experimental uncertainties in the values of C and Ω are relatively large, more precise measurements of the hyperfine intervals would certainly be desirable.

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